# Rafael R. Del Grande

Computational Material Scientist / Condensed Matter Physicist
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Personal Page | Google Scholar | GitHub | Linkedin | ORCID

## SKILLS

**Computational Materials Modeling**: DFT (Quantum Espresso, SIESTA, Octopus), Many-body perturbation theory (BerkeleyGW), Electron-phonon interpolation (EPW, Wannier90), Classical Molecular Dynamics (LAMMPS)
**Theoretical Physics:** Tight binding, Group Theory
**Software Development & Data Analysis**: Python (NumPy, Pandas, Matplotlib, Ploty, ASE, Jupyter), R, Bash, Mathematica
**Machine Learning**: TensorFlow, PyTorch, ScikitLearn, Optuna
**Languages**: Portuguese (Native), English (Fluent), Spanish (Intermediate), French (Basic)

## EXPERIENCE

**Postdoctoral Scholar** – University of California, Merced. Merced, CA *Jul 2021 - Present*

- Developed Python code that predicted excited-state forces, integrating quantum electron-phonon coupling with excitonic effects. Applied it to molecules, 1D, 2D, bulk, and defects
- Designed and automated high-performance simulation workflows combining DFT, DFPT and many-body methods
- Developed and trained Graph Neural Networks to predict GW corrections based on wavefunctions projections for monolayer $MoS_2$. Now working on predicting GW energy levels for supercells with sulfur vacancies
- Combined classical molecular dynamics and first-principles simulations to understand light-matter interactions in twisted 2D materials
- Predicted first and second order resonant Raman spectra for organic molecules and transition metal dichalcogenides
- Developed a scheme to accelerate large-scale BSE calculations, enabling simulations of systems with defects
- Mentored undergraduate summer research students

**Research Intern** – IBM. Rio de Janeiro, Brazil *Dec 2013 – May 2016*

- Performed molecular dynamics simulations of nanodroplets over silica surface to study relevant aspects of nanowetabillity to enhanced oil recovery
- Developed coarse-grained force field models enabling large-scale molecular dynamics simulations (up to 140 nm)
- Collaborated with studies of wettability that integrated different scale simulation methods (classical molecular dynamics and lattice Boltzmann) and experimental results

**Graduate Researcher** – Federal University of Rio de Janeiro. Rio de Janeiro, Brazil *Mar 2015 – Jun 2021*

- Investigated self-trapped excitons in carbon nanotubes with $sp^3$ defects visioning applications in quantum information
- Used genetic algorithm to fit tight binding parameters to perform electronic structure calculations of carbon nanotubes with random distributions of defects
- Performed DFT simulations and classical force field simulations of twisted multi-layer graphene

**Physics Lecturer** – Federal University of Rio de Janeiro. Rio de Janeiro, Brazil *Mar 2015 – Jun 2021*

## EDUCATION

**Ph.D. in Physics** (GPA 2.52/3.0) Mar 2017 - Jun 2021
Federal University of Rio de Janeiro. Rio de Janeiro, RJ, Brazil
Awarded *Bolsa nota 10* - excellence fellowship from FAPERJ (Rio de Janeiro state funding agency)
**M.Sc. in Physics** (GPA 2.45/3.0) Mar 2015 - Feb 2017
Federal University of Rio de Janeiro. Rio de Janeiro, RJ, Brazil
**B.Sc. in Nanoscience and Nanotechnology** (GPA 7.7/10.0) Mar 2011 – Feb 2015
Federal University of Rio de Janeiro. Rio de Janeiro, RJ, Brazil

## PUBLICATIONS

### *In production*

[19] Vk centers in LiF. **R. R. Del Grande**, D. A. Strubbe
[18] Ab initio first and second order resonant Raman of single and double wall zigzag carbon nanotubes. **R. R. Del Grande**, D. A. Strubbe
[17] First and second order resonant Raman with *ab initio* exciton-phonon interactions. **R. R. Del Grande**, D. A. Strubbe
[16] *Ab initio* exciton-phonon interactions of intralayer and interlayer excitons in bilayer $WSe_2$ and $MoS_2$. **R. R. Del Grande**, D. A. Strubbe
[15] Strain dependent exciton-phonon effects in orthorhombic, tetragonal and cubic methylammonium lead iodide perovskites. R. R. Del Grande, D. A. Strubbe
[14] BerkeleyGW-4.x: A portable exascale-ready software package for electronic excited-state properties of materials. M. Del Ben, Z. Li, F. H. da Jornada, D. Y. Qiu, D. A. Strubbe, D. Vigil-Fowler, A. Altman, B. A. Barker, A. Cepelloti, A. Chamapagne, Y. Chan, M. R. Filip, S. Gant , **R. R. Del Grande**, J. Harber, C. Hu, W. Huhn, O. Hull, W. Kim, M. H. Naik, C. S. Ong, S. Rafaely-Abramson, J. Ruan, W. Tang, P. Thomas, D. Weinberg, M. Wu, F. Zhao, F. Zhang, J. B. Neaton, J. R. Deslippe and S. G. Louie
[13] Consequences of H $sp^3$ doping in the electronical and optical properties of Carbon Nanotubes. **R. R. Del Grande**, D. A. Strubbe, M. G. Menezes, R. B. Capaz
[12] Anisotropic strain in low angle twisted bilayer $WSe_2$. **R. R. Del Grande**, D. A. Strubbe

### *Preprints*

[11] Revisiting excited state forces from many-body Green's function formalism: approximations and benchmark. **R. R. Del Grande**, D. A. Strubbe. https://doi.org/10.48550/arXiv.2502.05144
[10] Multi scale calculation of light-induced interlayer changes in low-angle twisted bilayer $WSe_2$. **R. R. Del Grande**, D. A. Strubbe. https://doi.org/10.48550/arXiv.2604.28143

### Published

[9] Highly Anisotropic Quasi-Direct Organic Metal Halide Hybrids: A Platform for Polarization-Sensitive Optoelectronics. R. Karkee, **R. R. Del Grande**, Y. Lee, J. Yoo, A. Ben-Akacha, B. Ma, M. T. Pettes, D. A. Strubbe. Advanced Materials Technologies, e02565 (2026) https://doi.org/10.1002/admt.202502565
[8] How to choose efficiently the size of the Bethe-Salpeter Equation Hamiltonian for accurate exciton calculations on supercells. **R. R. Del Grande**, D. A. Strubbe. Physical Review B, 112, 165118 (2025) https://doi.org/10.1103/dg13-y4kj
[7] Flat bands and gaps in twisted double trilayer graphene. F. J. Culchac, **R. R. Del Grande**, M. G. Menezes, R. B. Capaz. Physical Review B, 111, 075111 (2025) https://doi.org/10.1103/PhysRevB.111.075111
[6] Home experiments: a hands-on adaptation of the Experimental Physics II course at UFRJ for remote teaching. A. R. Hernández, A. M. Gomes, E. H.C.P. Sinnecker, **R. R. Del Grande**, R. B. Capaz and S. C. Cardoso. Rev. Bras. Ensino Fís. 43 (2021) https://doi.org/10.1590/1806-9126-RBEF-2021-0248 (*in Portuguese*)
[5] Flat bands and gaps in twisted double bilayer graphene. F. J. Culchac, **R. R Del Grande**, R. B. Capaz, L. Chico, E. S. Morell. Nanoscale 12, 5014-5020 (2020) https://doi.org/10.1039/C9NR10830K
[4] Energy barriers for collapsing large-diameter carbon nanotubes. **R. R. Del Grand**e, A. F. Fonseca and R. B. Capaz. Carbon 159 161-165 (2020) https://doi.org/10.1016/j.carbon.2019.12.030
[3] Layer breathing and shear modes in multilayer graphene: a DFT-vdW study. **R. R. Del Grande**, M. G. Menezes and R. B. Capaz J. Phys.: Cond. Matter 31 295301 (2019) https://doi.org/10.1088/1361-648X/ab1995
[2] From Nanoscale Wetting Towards Enhanced Oil Recovery. R. Giro, M. B. Steiner, P. W. Bryant, **R. R. Del Grande**, M. Engel. Offshore Technology Conference Brasil - 27-29 (2015) https://doi.org/10.4043/26232-MS
[1] Multi-scale modeling of wetting: effects of surface roughness. R. Giro, P. W. Bryant, M. B. Steiner, **Rafael R. Del Grande**, C. Feger, M. Engel. CILAMCE 2014 - XXXV Iberian Latin American Congress on Computational Methods in Engineering (2014)

## AWARDED COMPUTATION GRANTS

- Texas Advanced Computing Center (TACC) Frontera Pathways. Title: Ab initio excited-state forces from GW/BSE and DFPT calculations: applications to perovskites and 2D materials. Role: PI. Amount: 102,000 CPU/GPU Node Hours. Year: 2023-2025. Co-PI: David A. Strubbe.
- San Diego Supercomputer Center (through ACCESS). Title: Excited-state forces from GW/BSE and DFPT calculations. Role: PI. Amount: 10,000 CPU Node Hours and 93 GPU Node Hours. Year: 2022-2023. Co-PI: David A. Strubbe.
- Santos Dumont cluster at LNCC (Scientific Computing National Lab) in Rio de Janeiro, Brazil. Year: 2018-2021. Role: I helped my PhD advisor (Marcos G. Menezes) writing the proposal.

## MENTORING

(2023) Nathan Simons - Undergraduate student. Co-advised with Prof. David A. Strubbe. Senior thesis at UC Merced. Thesis title: Assessing the Accuracy of Vibrations in Machine Learning Potentials for Hydrogenated Amorphous Silicon
(2022) Onasis Mora - Undergraduate student. Co-advised with Prof. David A. Strubbe. Summer REU. Project title: Moiré patterns in twisted bulk layered materials

## TRAININGS

(2026) IBM AI Engineering. IBM on coursera.org
(2026) Data Science: Statistics and Machine Learning. Johns Hopkins on coursera.org
(2025) Artificial Intelligence for Materials Science. NIST, Maryland.
(2025) Teaching Strategies that Work: FTI Workshop for Educators. American Physical Society.
(2025) Deep Learning Specialization. DeepLearning.AI on coursera.org
(2025) Machine Learning Specialization. Stanford University & DeepLearning.AI on coursera.org
(2024) Machine Learning Summer Institute. Texas Advance Computing Center, University of Texas, Austin.
(2022) School on Electron-Phonon Physics from First Principles. University of Texas, Austin.
(2022) 9$^{th}$ Time-dependent Density Functional Theory: Prospects and Applications. Benasque, Spain.
(2022) Level 2: Principles of Pedagogy. University of California, Merced.
(2022) 2$^{nd}$ Mobile Summer Institute on Scientific Teaching (MoSIST). University of California, Merced.
(2021) 7$^{th}$ BerkeleyGW Tutorial (2021) Workshop. Online
(2021) Excited States and Nonadiabatic Dynamics CyberTraining Workshop. University at Buffalo SUNY. Online
(2018) XVI Brazilian School of Electronic Structure. Brazilian Physical Society. Santa Maria, RS, Brazil
(2016) XV Brazilian School of Electronic Structure. Brazilian Physical Society. São Bernardo do Campo, SP, Brazil
(2015) AFM principles, Federal University of Rio de Janeiro. Rio de Janeiro, Brazil.

## VOLUNTEER EXPERIENCE

***Volunteer* Physics Teacher** | Rio de Janeiro, RJ, Brazil |**Apr/2017–Aug/2019**
Preparatory physics classes for low-income high-school students for National Exams used in universities' admissions in Brazil

## PEER REVIEWING

Physical Review Letters, Physical Review B, Physical Review Materials, Nature Communications, Journal of Physics and Chemistry of Solids, Europhysics Letters, Chemical Physical Letters, The Journal of Physical Chemistry

## AFFILIATIONS

- Brazilian Physical Society 2015, 2017-2021
- American Physical Society 2017, 2021-2026

## CONFERENCES AND WORKSHOPS

### Presentations

#### Invited (Total = 1)

(2022) Excited state forces from GW/BSE and DFPT calculations. Rafael R. Del Grande, David Strubbe. 9$^{th}$ Time-Dependent Density-Functional Theory: Prospects and Applications. Benasque, Spain.

#### Contributed (Total = 14)

(2026) Ab initio calculation of light-induced structural changes in low-angle twisted bilayer $WSe_2$. Rafael R. Del Grande, David Strubbe. APS March Meeting, Denver, CO, USA
(2025) Ab initio excited state forces in the study of self-trapped excitons and coherent phonon generation. Rafael R. Del Grande, David Strubbe. APS March Meeting, Anaheim, CA, USA
(2024) Ab initio excited state forces in the study of self-trapped excitons and coherent phonon generation. Rafael R. Del Grande, David Strubbe. APS March Meeting, Minneapolis, MN, USA
(2023) Excited-state force calculations from GW/BSE and DFPT: development and application to organic metal halide perovskites. Rafael R. Del Grande, David Strubbe. APS March Meeting, Las Vegas, NV, USA
(2022) Excited-state forces in organic metal halide perovskites from GW/BSE calculations Rafael R. Del Grande, David Strubbe. APS March Meeting. Chicago, IL, USA
(2021) Effect of $sp^3$ defects covalent bonding in the optical absorption and electronic structure of carbon nanotubes. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. Encontro de Outono SBF. Online
(2021) Effect of defects covalent bonding in the optical absorption and electronic structure of carbon nanotubes. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. APS March Meeting. Online
(2019) Energy barrier for carbon nanotube collapse. Rafael R. Del Grande, Alexandre F. Fonseca, Rodrigo B. Capaz. Encontro de Outono SBF. Aracaju, SE, Brazil
(2017) Energy Barrier for Carbon Nanotube Collapse. Rafael R. Del Grande, Rodrigo B. Capaz. 18th International Conference on the Science and Application of Nanotubes and Low-dimensional Materials. Belo Horizonte, MG, Brazil
(2017) Energy Barrier for Carbon Nanotube Collapse. Rafael R. Del Grande, Rodrigo B. Capaz. APS March Meeting. New Orleans, LA, USA
(2017) Influence of Van der Waals corrections on multi-layer graphene/graphite systems in Density Functional Theory. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. XL Encontro Nacional da Física da Matéria Condensada. Búzios, RJ, Brazil
(2016) Shape Transitions of Carbon Nanotubes Using Molecular Dynamics. Rafael R. Del Grande, Rodrigo B. Capaz. VI Encontro do INCT de Nanomateriais de Carbono. Curitiba, PR, Brazil

(2014) Estudo computacional da dinâmica conformacional dos nanotubos de carbono. Rafael R. Del Grande, Rodrigo B. Capaz. XXXVI Jornada Giulio Massarani de Iniciação Científica, Tecnológica, Artística e Cultural. Rio de Janeiro, RJ, Brazil
(2013) Estudo do colapso de Nanotubos de Carbono por Dinâmica Molecular. Rafael R. Del Grande, Rodrigo B. Capaz. XXXV Jornada Giulio Massarani de Iniciação Científica, Tecnológica, Artística e Cultural. Rio de Janeiro, RJ, Brazil

### Poster (Total = 13)

(2026) Ab initio calculation of light-induced structural changes in low-angle twisted bilayer $WSe_2$. Rafael R. Del Grande, David Strubbe. Total Energy Workshop. Berkeley, CA, USA
(2025) Accelerating excited-state relaxations with Neural Networks. Rafael R. Del Grande, David A. Strubbe. Artificial Intelligence for Material Science Workshop. NIST. Rockville, MD, USA
(2024) Ab initio excited state forces towards light-induced changes in methylammonium lead iodide perovskites. Rafael R. Del Grande, David Strubbe. APS March Meeting, Minneapolis, MN, USA
(2023) Excited-state force calculations from GW/BSE and DFPT: development and application to organic metal halide perovskites. Rafael R. Del Grande, David Strubbe. 35th Workshop on Recent Developments in Electronic Structure Methods. Merced, CA, USA
(2022) Excited state forces from GW/BSE and DFPT calculations. Rafael R. Del Grande, David Strubbe. School on Electron-Phonon Physics from First Principles. Austin, TX, USA
(2022) Effect of $sp^3$ defects covalent bonding in the optical absorption and electronic structure of carbon nanotubes. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. APS March Meeting. Chicago, IL, USA
(2021) Consequences of H Doping in the Electronic and Optical properties of Carbon nanotubes. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. 35$^{th}$ Workshop on Recent Developments in Electronic Structure Methods. Online
(2020) Effect of hydrogen covalent bonding in the optical absorption and electronic structure of carbon nanotubes. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. Encontro de Outono SBF. Online
(2019) Absorption spectra of carbon nanotubes with $sp^3$ defects. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. Graphene Brazil. Rio de Janeiro, RJ, Brazil
(2018) Influence of Van der Waals corrections on multi layer graphene/graphite systems in Density Functional Theory. Rafael R. Del Grande, Marcos G. Menezes, Rodrigo B. Capaz. Encontro de Outono SBF. Foz do Iguaçu, PR, Brazil
(2016) Shape Transitions of Carbon Nanotubes Using Molecular Dynamics. Rafael R. Del Grande, Rodrigo B. Capaz. VI Encontro do INCT de Nanomateriais de Carbono. Curitiba, PR, Brazil
(2015) Shape transitions of carbon nanotubes using molecular dynamics. Rafael R. Del Grande, Rodrigo B. Capaz. XIV Brazilian MRS Meeting. Rio de Janeiro, RJ, Brazil.
(2015) Shape transitions of carbon nanotubes using molecular dynamics. Rafael R. Del Grande, Rodrigo B. Capaz. XXXVIII Encontro Nacional de Física da Matéria Condensada. Foz do Iguaçu, PR, Brazil

### Collaborated as instructor

(2023) 9$^{th}$ BerkeleyGW Tutorial Workshop and 4$^{th}$ Berkeley Excited States Conference (BESC2023). Oakland, CA, USA.
(2022) 9$^{th}$ Time-Dependent Density-Functional Theory: Prospects and Applications. Benasque, Spain.
(2022) 8$^{th}$ BerkeleyGW Tutorial Workshop and 3$^{rd}$ Berkeley Excited States Conference (BESC2022). Online.
(2015) Simulação Computacional de Sistemas Moleculares. Rio de Janeiro, RJ, Brazil.

## Attendence

(2014) IV Jornada de Nanotecnologia. Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil
(2013) III Jornada de Nanotecnologia. Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil
(2012) II Jornada de Nanotecnologia. Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil
(2011) I Jornada de Nanotecnologia. Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil